2. MATERIALS DEVELOPMENT

A. Integrated Approach for Development of Energy-Efficient Steel Components for Heavy Vehicle and Transportation Applications

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Objective

- This project focuses on development of methods and tools to achieve energy-efficient and environmentally benign steel components. The primary objective of this four-year project is to develop microstructure-level (often called mesoscale) simulation tools to capture the formation and influence of nonhomogeneous (real life) microstructures in steel processing. The tools will be used to understand and predict microstructure evolution during processing and ultimately to predict the resultant component performance. This information will then be used to design steel microstructures and develop process roadmaps. The developed techniques will be demonstrated on a pilot project at Caterpillar involving a defined structural component, namely a track roller shaft, which represents a steel component with high production volume that can potentially benefit from microstructure-level improvements. These goals will be achieved through the four tasks described in the technical task section.

Approach

To apply an integrated approach to development of energy-efficient steel components, three major areas of research needs will be pursued:

- Develop microstructure-level models to accurately predict the evolution and behavior of steel microstructures during component processing and performance.
- Characterize thermo-mechanical properties of microstructural constituents as a function of temperature and composition for exact chemistries.
- Develop the tools to assess required environmental resources and integrate them into the modeling simulation endeavor.

Accomplishments

- Reviewed project objectives and task responsibilities of each participating organization at the project kick-off meeting in September 2003.
- Distributed the two alloys to be investigated to the project team members so that machining of the test specimens required for the microstructural characterization, machining experiments, and strain rate dependent mechanical property determination tasks could be initiated during the first quarter of FY 2004.

Future Direction

During the first year, work will begin on all of the tasks described in the technical tasks section in this report; the project participants will also demonstrate that the approach and methods are valid. To this end the project will focus on Task 2, Machining Processing, and Task 4, Pilot Project, and will use parts of the work described in these tasks as a proof of concept. More specifically, our first year deliverables will be the following:

- Select a 1500-series steel and a micro-alloyed steel that are typical of track roller shaft applications, identifying the microstructures that are most commonly used for these applications.
- Produce and characterize the microstructures in the laboratory for both types of steel.
- Perform all mechanical tests on these microstructures that are required for inputs and validation of the mechanical models. These tests will include the temperature and strain rate dependence of mechanical properties. In addition, fracture toughness will be measured for these microstructures.
- Model the mechanical tests all the way through plastic deformation and fracture to determine actual material response. The simulation results will be validated using measured stress-strain curves and fracture toughness for the selected microstructures.
- Create a basic machining model from these models and demonstrate its applicability to one machining process of a 1500-series steel and a micro-alloyed steel for a track roller shaft. The orthogonal machining tests will be conducted using two cutting speeds and two depths of cut for a 1500-series steel and a micro-alloyed steel. The chip morphologies will be characterized and used for model validation.

Introduction

Product cost and performance are two major pressures influencing the acceptance of energy savings technologies by the manufacturers, suppliers, and users in the heavy vehicle and transportation industries. Energy cost has become a significant portion of total product cost for steel applications. Major reductions in energy use are potentially achievable for the transportation and heavy vehicle industries through development and optimization of cost-effective fabrication processes and enhanced product performance. The key enabling technologies to achieve these benefits are improved materials and realistic, microstructure-level simulations to predict manufacturability and life-cycle performance. Over the past two decades, steel mills and forge shops have successfully implemented numerous energy-efficient processes. The next logical step is to focus on the development of steel microstructures that are produced in such a way that they are energy efficient and environmentally benign over the entire manufacturing cycle.

Structural materials used in critical steel components of machines have evolved to the point where further improvements in the performance can be achieved only through a fundamental understanding of the mechanisms driving material behavior during processing and service. Microstructural elements such as grain size, inclusion and precipitate distributions, and chemistry control the performance of engineering materials. Variation in these microstructural elements leads to variation in such critical properties as fatigue life, toughness, and wear resistance. Therefore, understanding and developing the capability to control the formation of steel microstructures and predicting its functional and environmental performance is critical to moving the industry closer to its energy-efficiency, resource-efficiency, and pollution-prevention goals. The full realization of these benefits, however, requires a design tool that optimizes the microstructure with respect to the mechanical and environmental performance throughout the life cycle of a particular steel component.

To apply an integrated approach to development of energy-efficient steel components, the development of three major areas of research needs to be completed:

- microstructure-level models to accurately predict evolution and behavior of steel microstructures during component processing and performance,
- thermomechanical properties of microstructural constituents as a function of temperature and composition for exact chemistries, and
- tools to assess required environmental resources.

This project addresses activities required for the first of these three areas. The second and third tasks are either supported by current funding through the National Science Foundation or are expected to be funded through the DOE Initiative for Proliferation Prevention. Through these integrated efforts, a design tool will be developed that optimizes the microstructure, manufacturability, and performance of components with respect to the mechanical and environmental performance required throughout the components' life cycles. The overall benefit of this research will be the development and demonstration of a design methodology that will enable the domestic transportation and heavy vehicle industries to compete effectively in future worldwide markets through improved product performance and energy savings. Furthermore, the proposed design tool can be extended to other materials, i.e., cast iron, aluminum, titanium, magnesium, nickel-based alloys, ceramics, and composites, thus impacting virtually all industries.

In addition to the transportation and steel industries receiving significant energy and cost savings benefit through microstructure-level modeling, virtually all industries will be impacted. Examples of such industries include aerospace (engines, transmissions, structural), marine (engines and drives), agricultural and construction equipment, oil and chemical processing (pumps and gear boxes), military vehicles, mining machinery, appliances (compressors, motors, gear boxes, shafts), power tools, and automotive aftermarket.

Deliverables

The deliverables for the project will be the following:

- Microstructure-level methods for simulating the manufacturing cycle of steel products coupled with material performance computations (Tasks 1, 2, and 3).
- A specific chemical composition and processing map for a 1500-series steel and a micro-alloyed steel suitable for the application under consideration (Task 4).
- Energy and environmental resources required to produce the selected steel component using at least two steels and processing schemes (Task 4).

The project tasks will focus on three critical areas in the development of these models: heat treatment processing, machining, and materials performance in specific applications. These three processes have been chosen because they are critical steps in reaching the goal of being able to develop a specific steel for a particular application with a heavy reliance on modeling and with energy requirements optimized as an integral part of the development process. Modeling of casting and forming processing has been performed under other programs, and Caterpillar has shown successful application and commercialization of these models. These existing models will be used along with the heat treatment, machining, and specific applications models described below to complete a suite of models for the manufacture of micro-alloyed steels.

To accomplish the project objectives, a multidisciplinary team consisting of a national laboratory, a university, and a steel end user has been assembled. The team will be supported by an international research institute for material characterization and by experts in environmental impact assessment. The section below describes each of the technical tasks to be performed.

Technical Tasks

Task 1: Heat Treating Process

This task will quantify the influence of chemical and microstructural inhomogeneities in the austenite phase on the final heat-treatment response. The microstructure-level models incorporating phase transformation kinetics, polycrystalline plasticity, and recrystallization dynamics will be developed collaboratively by the Oak Ridge National Laboratory (ORNL), Brown University, and Caterpillar. Validation will be accomplished using the unique experimental capabilities and expertise at ORNL for conducting kinetic and metallurgical characterization as well as utilizing Caterpillar's ability to produce heat-treated specimens in precisely specified and controlled conditions. The modeling effort will draw on the significant programs at Brown and Caterpillar that have developed microstructural modeling capabilities.

The coupled mesoscale deformation and recrystallization models developed cooperatively by the three team members will be implemented to study the influence of mill thermomechanical processing variables and mesoscale composition variation on the grain size, grain-size distribution, and austenite grain-boundary character prior to the decomposition of austenite. The coupled deformation and recrystallization models will be used to predict the evolution of austenite grain structure and grain-boundary character distribution during the thermomechanical processing steps involved during secondary fabrication. The output of these simulations will directly feed into an austenite decomposition code that predicts phase transformation during the heat-treatment operation.

The austenite decomposition code will be a microstructure-level tool, which accounts for alloying element concentration within each grain and grain boundary. For validating the austenite decomposition tool, several experimental techniques will be employed. High-speed quenching dilatometry, high-resolution scanning transmission electron microscopy, and X-ray synchrotron diffraction capabilities at ORNL will be used to quantify the fine (~10 nm to 8 μm) microstructural features that evolve during the various phase transformation sequences in steels. In particular, microanalyses will be performed to characterize any chemical inhomogeneity that might arise as a result of solute partitioning from the solidified microstructure.

Task 2: Machining Processing

A microstructure-level model will be applied to machining simulation of steels to determine their machinability and material state after thermomechanical processing. The model will consist of four main elements integrated into the finite element structure: microstructure simulation, material modeling, material characterization, and material flow and fracture. The microstructure simulation module will assemble individual constituents into a composite material based on microstructural composition, grain size, and grain-size distribution. This information along with residual stress predictions for individual grains will be obtained from Task 1. The material modeling module will account for the response of each constituent to high strains, strain rates, temperature, damage, and effects of loading paths associated with machining. The material characterization part will provide the material modeling module with parameters to define strain rate and temperature-dependent behavior of individual phases. The material flow and fracture module will periodically examine each grain for damage, locate deformed grain boundaries, and generate new boundaries. This module will compute stress, strain, temperature, and damage in each phase based on initial microstructure, material state, tool geometry, and process parameters.

The overall model will be developed collaboratively by Caterpillar and Brown University. Both institutions have strong reputations for machining models that incorporate microstructural elements into the models. The mechanical testing will be performed at Brown University, which has the capability to test samples over a wide range of strain rates in compression, tension, and torsion. Brown University also has the ability to perform jump tests in which the strain rate is changed during the deformation process to ascertain the strain rate sensitivity behavior of each chemistry and microstructure combination.

The microstructural analysis will be performed both at ORNL and at Brown University. At Brown, the primary methods that will be used to examine microstructure will be optical metallography and scanning electron microscopy (SEM). The SEM will be performed on a LEO-1530VP field emission instrument that has a resolution of 1 nm at an incident beam voltage of 20 kV. This instrument is fully equipped with energy dispersive X-ray analysis for chemical composition determination. As needed, the material characterization tasks at ORNL will include SEM, transmission electron microscopy, X-ray and neutron diffraction phase identification and residual stress measurements, and phase transformation kinetic and dilation dilatometry. Available resources will include the Hitachi HD-2000 STEM with SEM, STEM, and Z-contrast imaging capability; the PHI 680 Scanning Auger Microprobe with high sensitivity to light elements; the JEOL 8200 electron Superprobe; and the MMC High Speed Quenching and Deformation Dilatometer. A significant benefit of the majority of these resources is that these instruments can be operated remotely from outside ORNL so that the collaborating team can interact and interpret results in real-time for these characterization endeavors. Any X-ray (including synchrotron) and neutron diffraction analyses required for this project will leverage the capabilities of the ORNL High Temperature Materials Laboratory Diffraction and Residual Stress Centers. These facilities have unique state-of-the art equipment that enable both room temperature and elevated temperature characterizations to be made up to 2700ºC in vacuum and 1600ºC in air. In addition, ORNL's High Flux Isotope Reactor's Neutron Diffraction Center enables nondestructive depth profiling of macro and micro residual stresses in rather large bulk specimens.

A concerted effort will be made to review and leverage all current developments in this material and process simulation field that is the scope of this project. Microstructure, residual stress, and cutting force measurements obtained by various research groups (e.g., ongoing research at Purdue University by S. Chandrasekar) will be used for model development and validation.

Task 2 as well as Task 1 will be augmented by a parallel project between Caterpillar, Brown, and the Central Research Institute for Materials in St. Petersburg, Russia, in which a detailed examination is being performed on the relationship between composition, microstructure and mechanical properties on steels of highly controlled purity and microstructure.

Task 3: Material Performance and Application

After the materials have been processed and machined, the next concern is to predict their subsequent performance, that is, their strength and resistance to fracture. Thus, the models for material performance need to be developed and validated. These models will explicitly include such microstructural elements as inclusions, precipitates, and grain boundaries and will be based on several finite element methods developed at Brown University.

The first step will be to develop predictive models of damage initiation either by cracking or debonding of second-phase inclusions and precipitates. This modeling will be performed using a cohesive surface framework to model the interface between the inclusion (or precipitate) and the matrix and to model the initiation and growth of cracks within the second phase. Parameter studies will be undertaken to identify measurable and controllable features of the microstructure that are key for damage initiation. The results for damage initiation will be used in a modified Gurson model[1] to predict material performance. Of initial interest will be the prediction of performance in a suite of test specimens that give rise to different plastic strain-stress triaxiality histories so that the predictive capabilities of this modeling can be compared with experimental observations. Three-dimensional calculations of more complex geometries will also be performed to demonstrate the capability of predicting failure in component-like geometries.

At the same time, experiments will be performed that use specimens that have been carefully designed so that their mechanical response can be fully modeled. These specimens will be pulled in tension to various loads and then sectioned so that the microstructure can be observed. Particular attention will be given to identification of the second-phase particles that are present in the material and participate in crack nucleation. This examination will be performed at Brown University using the LEO 1530VP SEM described in the previous task. By performing serial sectioning of the sample and by making maps of the location of particles and determining whether the particles have cracked, debonded, or remained whole and intact, the details of the

[1] A.L. Gurson, "Continuum Theory of Ductile Rupture, Void Nucleation and Growth," *Journal of Engineering Materials Technology*, **99**, (2) (1977).

interactions between the microstructure and mechanics will be determined.

Task 4: Pilot Project

The proposed research will focus on track roller shafts as a pilot component. The track roller shaft represents a component with high production-volume steel at Caterpillar. It serves to transmit the weight of a tractor through the undercarriage (see Figure 1), and can be produced from either conventional steel (heat-treated for strength) or microstructurally improved "micro-alloy" steel. The use of micro-alloy steel has been demonstrated to reduce the cost and environmental impact of the heat-treatment stage, making it currently the preferred material in regions with high energy costs (such as Japan). The use of microstructure-level simulation and sustainability metrics to evaluate and optimize its environmental performance throughout the entire life cycle may lead to further improvements and serve as an example on the effectiveness of integrated methodology.

First, the entire life cycle of a track roller shaft made with a conventional 1500-series steel will be modeled, and environmental resources needed throughout a component life cycle will be assessed. The chemical composition and processing map will be optimized to minimize environmental impact and cost of the component. Then, the modeling process will be repeated for using a micro-alloyed steel, which will be optimized for the same requirements. This study aims to provide optimum chemical compositions and processing road maps for a track roller shaft made with a conventional 1500-series steel and a micro-alloyed steel. In addition, the pilot project will quantify energy and environmental resources required for the entire life cycle of a track roller shaft made with steels and processes mentioned above.

A critical component in this task as well as the others will be the quantification of energy use during production of a part and optimization of the proposed process to minimize energy usage. Caterpillar has already established a project called Bridges to Sustainability, and National Science Foundation (NSF) interns at Brown worked in the summer of 2003 on this project. The tools developed by the NSF-sponsored project will be applied in this project to assess energy usage and savings for the processes used here.

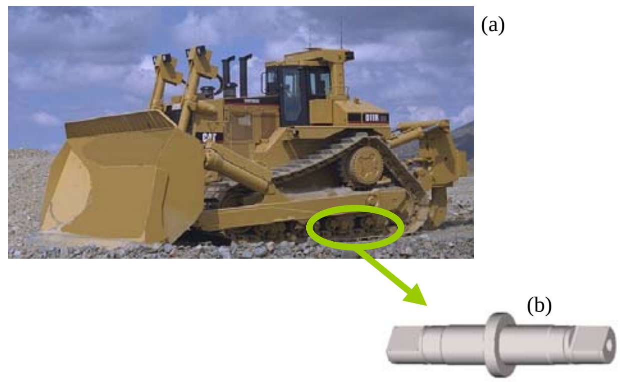

Figure 1. The tractor undercarriage receives the weight of the tractor (a) through a track roller shaft (b).